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Some first order exchange approximations in the calculation of total excitation cross-section of Li and Na by electron-impact

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Some first-order exchange approximations, namely, Ochkur, Ochkur-Rudge (OR), and Ochkur-Rudge-Bely (ORB) have been compared by using them to calculate the total excitation cross-section for some transitions in Li ($2s$–$2p$, $2s$–$3s$, $2s$–$3p$, $2s$–$3d$) and Na ($3s$–$3p$, $3s$–$3d$) by electronic impact. Ochkur-Rudge method is found to enhance the cross-section near the peak while ORB is found to lower it compared to the first Born approximation (FBA).

1. Introduction

In this paper we present the results of total integral cross-sections for some excitations of Li and Na by electron-impact calculated in the Ochkur approximation (Ochkur 1964) and in its two modifications by Rudge (1965) and by Bely (1966, 1967) and compare these results. A similar comparison of these and some other first-order methods has been done by Truhlar *et al* (1968) by applying them to $1s$–$2s$ excitation of hydrogen by electronic impact. They conclude that although these methods yield poor results for the differential cross-section, the results for integral cross-sections are quite good. We feel that further investigation is needed to assess the relative merits of these methods in the calculation of the integral cross-sections. Though Ochkur approximation-results for excitation of alkali metal atoms are available (Felden *et al* 1971, Greene *et al* 1974) but OR and ORB results for these are not available in the literature. We have, therefore, calculated the total integral cross-sections in these approximations for some excitations in Li ($2s$–$2p$, $2s$–$3s$, $2s$–$3p$, $2s$–$3d$) and Na ($3s$–$3p$, $3s$–$3d$) using two different types of wave functions. We have also calculated the FBA and Ochkur cross-sections. These provide a check on the accuracy of the calculations as well as the wave-functions used and facilitate an accurate comparison.

Our FBA cross-sections are found to be in reasonable agreement with those of Vainshtein *et al* as quoted by Moiseiwitsch *et al* (1968) and Greene *et al* (1974). Small differences, however, are due to the use of different wave-functions. We have used two types of wave-functions viz. Slater wave-functions suggested by Simsic *et al* (1972) and HF wave-functions due to Weiss (1963) for Li and due to

Szasz *et al* (1967) for Na ($3s$–$3p$). For Na ($3s$–$3d$) the ground state wave-function is due to Szasz *et al* (1967) while the excited state wave-function is due to Weiss. Calculations were performed with the help of computer at I.I.T., Kanpur.

2. Theory

Assuming a single active electron, the cross-section for excitation of an alkali metal atom from the initial state $(n_0 l_0)$ to the final state $(n_1 l_1)$ in the FBA is given (in atomic units) by

$$\sigma^{FBA} = \frac{8}{k_0^2} \sum_{\mu=|l_0-l_1|}^{l_0+l_1} C_\mu \int_{k_0-k_1}^{k_0+k_1} |F_\mu(q)|^2 q^{-3} dq \qquad \ldots (1)$$

where

$$C_\mu = (2\mu+1)(2l_1+1)\begin{pmatrix} \mu & l_0 & l_1 \\ 0 & 0 & 0 \end{pmatrix}^2 \qquad \ldots (2)$$

$$F_\mu(q) = \int_0^\infty P_{n_0 l_0}(r) P_{n_1 l_1}(r) j_\mu(qr) dr. \qquad \ldots (3)$$

$\begin{pmatrix} \mu & l_0 & l_1 \\ 0 & 0 & 0 \end{pmatrix}$ is the Clebsch-Gordon coefficient (Edmonds 1960), $j_\mu(qr)$ is the spherical Bessel function of order μ, $\boldsymbol{k}_0$ and $\boldsymbol{k}_1$ are the momenta of incident and scattered electron respectively and $\boldsymbol{q}$ is the momentum-transfer. $P_{nl}(r)$ are the radial functions of the active electron. The energy of the incident electron is written as $E = k_0^2$.

The earliest method to include the effect of exchange was Born-Oppenheimer method. An extensive study of this method by Bates *et al* (1950) revealed that the method was poor for rearrangement processes. Ochkur (1964) suggested to expand the exchange scattering amplitude in inverse powers of k_0 and to drop all the terms in the expansion except the first. Thus the exchange amplitude in Ochkur approximation is given by

$$g^0(\boldsymbol{k}_0, \boldsymbol{k}_1) = (q^2/k_0^2) f^B(\boldsymbol{k}_0, \boldsymbol{k}_1) \qquad (4)$$

where f^B is the Born direct amplitude. This leads to the total cross-section in the Ochkur approximation :

$$\sigma^0 = (8/k_0^2) \sum_{\mu=|l_0-l_1|}^{l_0+l_1} C_\mu \int_{k_0-k_1}^{k_0+k_1} (1 - q^2/k_0^2 + q^4/k_0^4) |F_\mu(q)|^2 q^{-3} dq \ldots (5)$$

Rudge (1965) has shown that expression (4) cannot be obtained from a variational expression. He modified the Ochkur result so that the scattering amplitude can be derived in a straight forward way from a variational expression. The Ochkur-Rudge exchange amplitude (Bely 1966) is given by

$$g^{0R}(\boldsymbol{k}_0, \boldsymbol{k}_1) = \exp(2i\phi_{01}) q^2/(U_0 + k_1^2) f^B(\boldsymbol{k}_0, \boldsymbol{k}_1) \qquad \ldots (6)$$

where

$$\phi_{01} = \text{arc } tg(\sqrt{U_0}/(k_0^2 + U_1 - U_0)).$$

U_0 and U_1 being the ionization energies in the initial and final states respectively. This leads to the total cross-section in OR approximation :

$$\sigma^{\mathrm{OR}} = (8/k_0^2) \sum_{\mu=|l_0-l_1|}^{l_0+l_1} C_\mu \int_{k_0-k_1}^{k_0+k_1} dq \left[1+q^4/(k_0^2+U_1)^2 - \frac{q^2 \cos 2\phi}{(U_1+k_0^2)} \right] \frac{|F_\mu(q)^2|^2}{q^3}$$

$$\phi = \text{arc } tg(\sqrt{U_0/(k_0^2-\epsilon)}) \qquad \ldots (7)$$

where ϵ is the threshold of excitation.

Bely (1966) has pointed out that though Born and Ochkur results satisfy the principle of detailed balance, OR result does not. To correct for this, he suggested replacing g^{OR} by its absolute value :

$$g^{\mathrm{ORB}} = |g^{\mathrm{OR}}|.$$

Thus in the ORB approximation,

$$\sigma^{ORB} = (8/k_0^2) \sum_{\mu=|l_0-l_1|}^{l_0+l_1} C_\mu \int_{k_0-k_1}^{k_0+k_1} [1+q^4/(k_0^2+U_1)^2 - q^2/(k_0^2+U_1)] \frac{|F_\mu(q)|^2}{q^3} dq. \qquad \ldots (9)$$

3. Results and Discussion

Total excitation cross-sections have been calculated using eqs. (1), (5), (7) and (9) for incident energies from 1·02 to 50 times the threshold of excitation. Integrations have been performed using Gauss-quadrature method. Table 1 shows the results of calculations. Results for only Slater wavefunctions are given for Li ($2s$–$2p$) and Li ($2s$–$3d$) while those for only Weiss wavefunctions are given for Li ($2s$–$3s$) and Li ($2s$–$3p$). The simple Slater wavefunctions are found to be quite satisfactory for Li, so far as these calculations are concerned. But for Na these yield poor results. Hence only the results of HF wavefunctions are reported for Na.

Recently some reliable experimental results for Li ($2s$–$2p$) by Leep & Gallagher (1974) and for Na ($3s$–$3p$) by Enemark & Gallagher (1972) have been reported and compared with various theoretical results. These comparisons show that the FBA exaggerates the cross-sections near the peak. For other cases reliable experimental results are not available (Walters 1976). A comparison of our results shows that OR cross-sections are somewhat (in some cases by more than 50%) higher than FBA near the peak. and hence, in worse agreement with experiments. Ochkur and ORB bring down the peak. The latter produces maximum lowering, though in no case it is more than 20%. For incident energies greater than 10 times the threshold, all these methods give nearly the same result which is also close to the FBA result. OR method not only enhances the peak but also shifts it to lower energy side. This is because the phase factor makes the interference term additive at lower incident energies.

Table 1. Total excitation cross-section in units of πa_0^2. Threshold of excitation, ϵ, is in Rydbergs.

Incident energy in threshold units	Li ($2s \rightarrow 2p$) $\epsilon = 0{\cdot}136$				Li ($2s \rightarrow 3s$) $\epsilon = 0{\cdot}2479$				Li ($2s \rightarrow 3p$) $\epsilon = 0{\cdot}2818$			
	FBA	OCHK	OR	ORB	FBA	OCHK	OR	ORB	FBA	OCHK	OR	ORB
1·02	41·89	42·00	60·89	32·62	1·21	1·20	2·39	0·936	0·997	1·01	2·20	0·804
1·04	57·77	58·04	83·55	45·22	1·66	1·63	3·21	1·29	1·35	1·38	2·49	1·10
1·08	77·82	78·36	111·40	61·52	2·22	2·13	4·10	1·74	1·74	1·82	3·73	1·45
1·16	100·40	101·00	140·80	80·79	2·81	2·61	4·82	2·24	2·07	2·20	4·29	1·78
1·32	120·50	119·60	162·50	99·69	3·27	2·88	4·95	2·66	2·18	2·29	4·15	1·92
1·64	129·60	124·30	163·50	111·40	3·36	2·84	4·31	2·80	1·94	1·89	3·14	1·70
2·28	121·70	112·00	140·00	108·70	2·94	2·50	3·23	2·53	1·45	1·27	1·23	1·23
3·56	99·36	90·84	104·10	91·68	2·16	1·92	2·17	1·95	0·935	0·785	0·972	0·787
6·12	71·88	67·56	71·69	68·24	1·38	1·28	1·34	1·29	0·544	0·474	0·516	0·477
11·24	47·44	45·87	46·77	46·06	0·789	0·757	0·768	0·759	0·299	0·274	0·282	0·275
21·48	29·43	28·96	29·11	29·00	0·425	0·417	0·418	0·417	0·159	0·151	0·153	0·152
30·00	22·85	22·60	22·66	22·62	0·308	0·303	0·304	0·303	0·115	0·111	0·111	0·111
20·00	15·56	15·47	15·48	15·47	—	—	—	—	—	—	—	—

Table 1—Contd.

Incident energy in threshold units	Li ($2s \rightarrow 3d$) $\epsilon = 0{\cdot}2658$				Na ($3s \rightarrow 3p$) $\epsilon = 0{\cdot}1545$				Na ($3s \rightarrow 3d$) $\epsilon = 0{\cdot}2658$			
	FBA	OCHK	OR	ORB	FBA	OCHK	OR	ORB	FBA	OCHK	OR	ORB
1·02	1·47	1·44	3·18	1·17	30·67	30·41	47·76	23·44	1·98	1·95	4·22	1·57
1·04	2·03	1·97	4·26	1·63	42·50	41·79	65·39	32·72	2·73	2·65	5·65	2·17
1·08	2·74	2·59	5·45	2·21	57·77	55·93	86·86	45·09	3·68	3·49	7·22	2·94
1·16	3·56	3·23	6·40	2·88	75·82	71·40	109·30	60·53	4·74	4·32	8·48	3·831
1·32	4·29	3·71	6·62	3·51	93·68	84·76	125·80	77·32	5·68	4·92	8·75	4·63
1·64	4·59	3·86	5·86	3·83	05·50	92·14	128·20	90·63	6·01	5·06	7·70	5·01
2·28	4·16	3·56	4·50	3·59	104·90	91·92	114·60	93·89	5·40	4·62	5·87	4·66
3·56	3·13	2·81	3·11	2·83	90·53	82·66	92·10	84·22	4·04	3·62	4·02	3·65
6·12	2·02	1·89	1·96	1·90	68·52	65·21	67·83	65·74	2·59	2·43	2·52	2·44
11·24	1·16	1·12	1·14	1·13	46·79	45·69	46·22	45·80	1·49	1·44	1·45	1·44
21·48	0·629	0·617	0·619	0·617	29·79	29·47	29·56	29·49	0·805	0·789	0·792	0·790
30·00	0·454	0·448	0·449	0·448	23·39	23·22	23·25	23·23	0·582	0·573	0·574	0·475
50·00	—	—	—	—	16·17	16·11	16·12	16·11	0·352	0·349	0·349	0·349

4. Conclusions

These methods provide simple means for the inclusion of exchange in a first-order theory, though none is completely satisfactory. OR method might be an improvement over Ochkur in calculating pure exchange cross-section as claimed by Truhlar *et al* (1968), but it is definitely not so in calculating total excitation cross-section. ORB provides some definite improvement over Ochkur at lower incident energies. At higher energies there is little difference between these.

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